

Analytical Approximation to the Local Softness and Hypersoftness and to their Applications as Reactivity Indicators

Supplementary Information

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Content:

1. Radial distribution functions of the density derivatives in 3s, 3p, 3d orbitals with the nuclear charges $Z=1$, $Z=2$ and $Z=3$.
2. Radial distribution functions for the electron density in 1s, 2s, 2p, 3s, 3p, 3d orbitals with nuclear charges $Z=1$, $Z=2$ and $Z=3$.
3. Collection of the extreme points in the radial density functions $\rho(r)$ and its derivatives under consideration in this work $f(r)$, $df(r)/dN$, $s(r)$, $ds(r)/dN$ for orbitals with nuclear charges $Z=1$, $Z=2$ and $Z=3$.

1. Radial distribution functions of the density derivatives in 3s, 3p, 3d orbitals

The complete body of derivatives discussed in this work has been presented in form of the radial distribution functions: $f(r)$, $df(r)/dN$, $s(r)$, $ds(r)/dN$ for the group of 3s, 3p and 3d orbitals, consecutively in Figures S1-S4. Each derivative has been calculated for three values of the atomic number ($Z=1$, $Z=2$, $Z=3$) distinguished by unified colors. Note the increasing scale on the ordinate axis when going from Figures S1 to S4; the scale is uniform in rows and has been marked in upper right corner of each diagram.

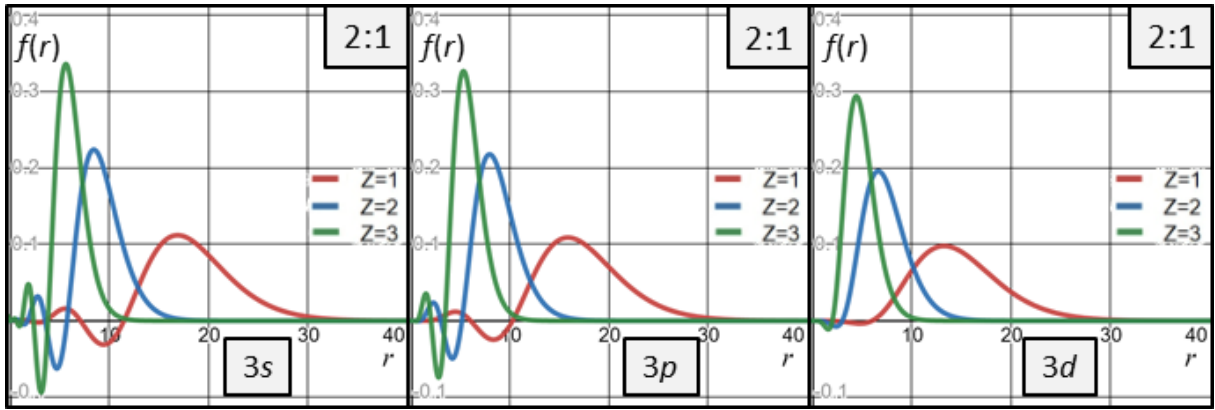


Fig. S1 Radial distribution for the Fukui function $f(r)$ for orbitals (Z -atomic number)

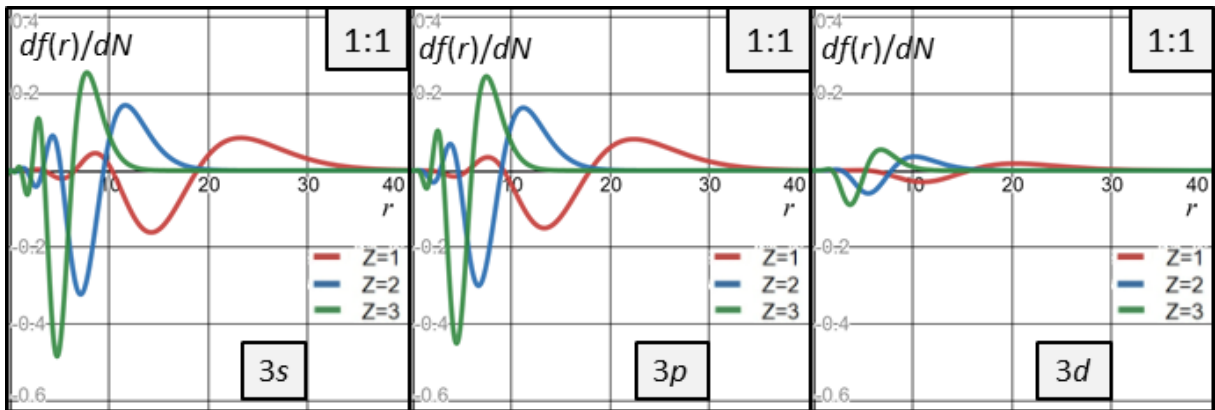


Fig. S2 Radial distribution for the derivative of the Fukui function $df(r)/dN$ for orbitals (Z -atomic number)

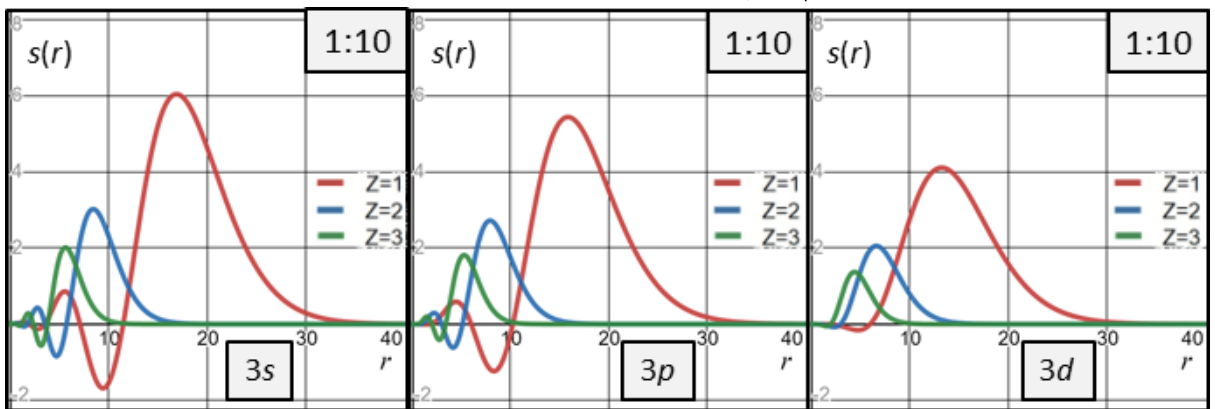


Fig. S3 Radial distribution function for the local softness $s(r)$ for orbitals (Z -atomic number)

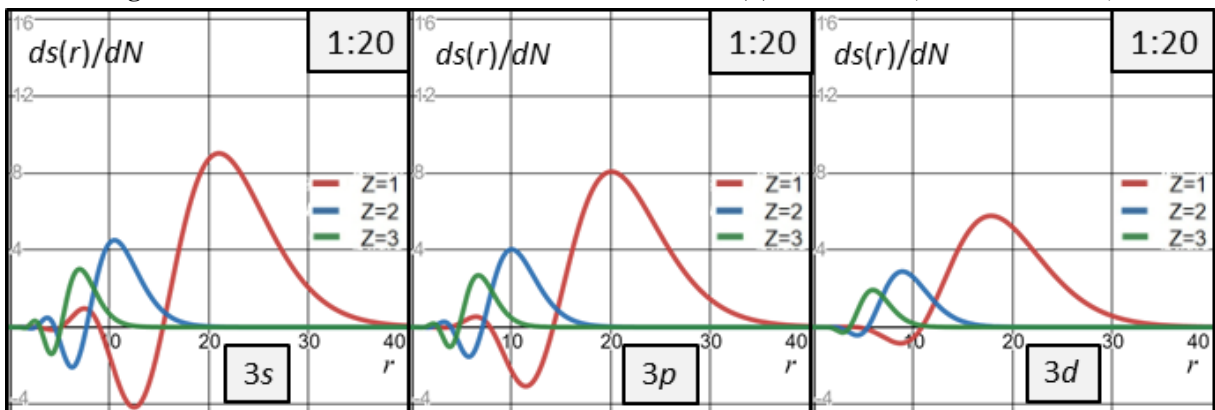


Fig. S4 Radial distribution for the derivative of the local softness $ds(r)/dN$ for orbitals (Z -atomic number)

2. Radial distribution functions for the electron density in 1s, 2s, 2p, 3s, 3p, 3d orbitals

The radial distribution function of the electron density has been presented for orbitals for three values of the atomic number ($Z=1, Z=2, Z=3$) distinguished by unified colors. The scale of pictures has been adjusted as to expose the details of all functions. The numerical data (the positions of the extreme values) have been collected separately (ref. p. 3).

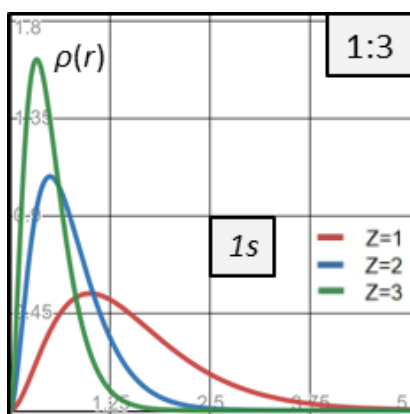


Fig. S5
Radial distribution of the electron density $\rho(r)$ for orbital 1s (Z -atomic number). The scale on ordinate axis has been contracted by 1:3 with respect to Fig. S6. Also note the shorter range on the ordinate axis with respect to Figures S6 and S7.

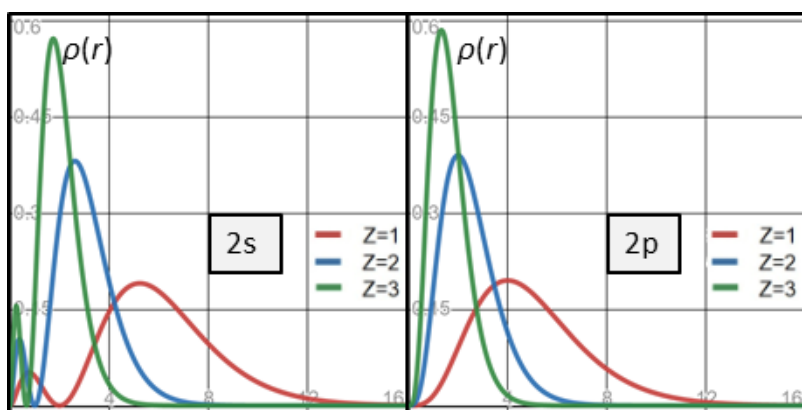


Fig. S6
Radial distribution of the electron density $\rho(r)$ for orbitals 2s and 2p (Z -atomic number)

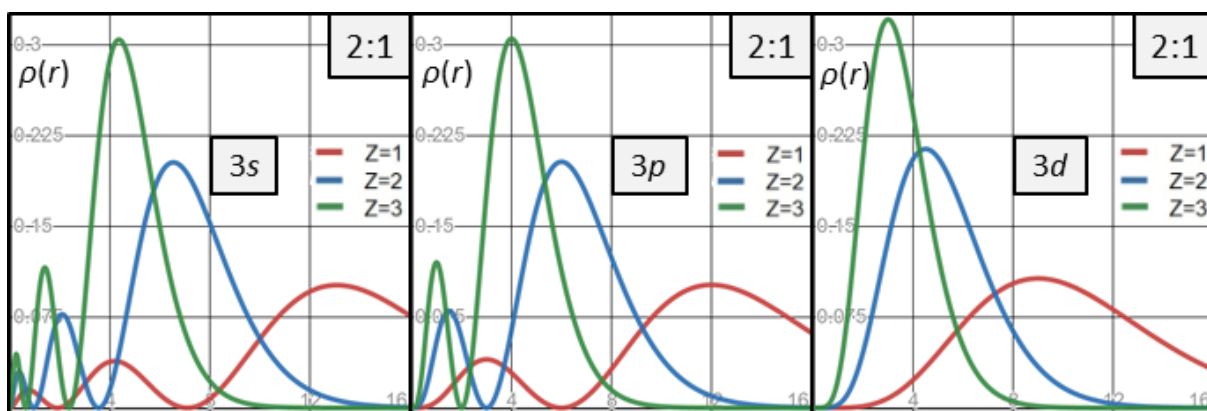


Fig. S7 Radial distribution of the electron density $\rho(r)$ for orbitals 3s, 3p and 3d (Z -atomic number). The scale on ordinate axis has been expanded by 2:1 with respect to Fig. S6.

3. Collection of the characteristic points in the radial distribution functions for the electron density $\rho(r)$ and its derivatives $f(r)$, $df(r)/dN$, $s(r)$, $ds(r)/dN$ as represented in Figures S1-S7.

Table S1

Characteristic points for the nuclear charge $Z=1$; max – maximum, min – minimum, mz – zero point
Distance r in a.u.

Z=1	Type	r	$\rho(r)$	Type	r	$f(r)$	Type	r	$df(r)/dN$	Type	r	$s(r)$	Type	r	$ds(r)/dN$
1s	max	1	0.5413	max	2	0.3907	min	1.581	-0.2399	max	2	2.3444	min	0.775	-0.036
							mz	2.791	0				mz	1	0
							max	4	0.1336				max	3.225	3.272
2s	max	0.764	0.0519	max	1.36	0.0077	min	1.301	-0.0105	max	1.36	0.185	min	0.7114	-1.027E-03
	min	2	0	mz	2	0	mz	1.893	0	mz	2	0	mz	0.8972	0
	max	5.236	0.191	min	3.135	-0.0215	max	2.899	0.0285	min	3.135	-0.516	max	2.262	0.103
				mz	4	0	mz	3.642	0	mz	4	0	mz	2.854	0
				max	7.505	0.1755	min	6.206	-0.214	max	7.505	4.211	min	4.917	-1.211
							mz	8.984	0	mz			mz	6.249	0
						max	11.689	0.1174	max			max	10.109	5.775	
3s	max	0.74	0.0148	max	1.306	0.00095	min	1.28	-0.00131	max	1.306	0.0515	min	0.699	-1.313E-04
	min	1.902	0	mz	1.902	0	mz	1.856	0	mz	1.902	0	mz	0.879	0
	max	4.186	0.0387	min	2.843	-0.00234	max	2.743	0.003149	min	2.843	-0.1265	max	2.121	0.01221
	min	7.098	0	mz	3.531	0	mz	3.386	0	mz	3.531	0	mz	2.636	0
	max	13.074	0.1015	max	5.56	0.01588	min	5.209	-0.0208	max	5.56	0.8578	min	4.239	-0.137
				mz	7.098	0	mz	6.536	0	mz	7.098	0	mz	5.121	0
				min	9.426	-0.03118	max	8.584	0.0451	min	9.426	-1.6835	max	7.479	0.967
				mz	11.469	0	mz	10.274	0	mz	11.469	0	mz	9	0
				max	16.866	0.11179	min	14.224	-0.161	max	16.866	6.037	min	12.474	-4.161
							mz	18.851	0	mz			mz	15.364	0
						max	23.234	0.0848	max			max	20.989	9.016	
2p	max	4	0.1954	min	1.551	-0.0018	max	1.476	0.0025	min	1.551	-0.036	max	1.0444	0.0007843
				mz	2	0	mz	1.889	0	mz	2	0	mz	1.268	0
				max	6.449	0.1636	min	5.255	-0.189	max	6.449	3.272	min	3.74	-0.332
							mz	8.055	0				mz	4.732	0
						max	10.838	0.1126				max	9.215	4.524	
3p	max	3	0.0401	min	1.378	-0.00017	max	1.3505	0.000232	min	1.3776	-0.00835	max	0.9492	7.208E-05
	min	6	0	mz	1.757	0	mz	1.7176	0	mz	1.757	0	mz	1.1459	0
	max	12	0.1018	max	4.463	0.011769	min	4.203	-0.0154	max	4.463	0.5885	min	3.12	-0.02947
				mz	6	0	mz	5.557	0	mz	6	0	mz	3.804	0
				min	8.316	-0.0247	max	7.593	0.0344	min	8.316	-1.233	max	6.437	0.539
				mz	10.243	0	mz	9.198	0	mz	10.243	0	mz	7.854	0
				max	15.844	0.1087	min	13.307	-0.1497	max	15.844	5.435	min	11.447	-3.066
							mz	17.936	0				mz	14.196	0
						max	22.367	0.0816				max	20.048	8.062	
3d	max	9	0.1071	min	4.757	-0.00371	max	4.447	0.00124	min	4.757	-0.156	max	3.478	0.008929
				mz	6	0	mz	5.543	0	mz	6	0	mz	4.146	0
				max	13.243	0.09778	min	10.979	-0.02968	max	13.243	4.107	min	8.722	-0.8386
							mz	15.673	0				mz	10.854	0
						max	20.296	0.01811				max	17.8	5.772	

Table S2Characteristic points for the nuclear charge $Z=2$; max – maximum, min – minimum, mz –zero point.Distance r in a.u.

Z=2	Type	r	$\rho(r)$	Type	r	$f(r)$	Type	r	$df(r)/dN$	Type	r	$s(r)$	Type	r	$ds(r)/dN$
1s	max	0.5	1.0827	max	1	0.7815	min	0.791	-0.4799	max	1	1.1722	min	0.388	-0.0178
							mz	1.396	0				mz	0.5	0
							max	2	0.2672				max	1.612	1.6358
2s	max	0.382	0.1038	max	0.68	0.0155	min	0.651	-0.021	max	0.68	0.093	min	0.3557	-5.136E-04
	min	1	0	mz	1	0	mz	0.947	0	mz	1	0	mz	0.4486	0
	max	2.618	0.3819	min	1.568	-0.043	max	1.449	0.057	min	1.568	-0.258	max	1.131	0.052
				mz	2	0	mz	1.821	0	mz	2	0	mz	1.427	0
				max	3.752	0.3509	min	3.103	-0.428	max	3.752	2.105	min	2.458	-0.605
							mz	4.492	0				mz	3.125	0
						max	5.845	0.2348				max	5.055	2.887	
3s	max	0.37	0.0297	max	0.653	0.00191	min	0.64	-0.00262	max	0.653	0.0258	min	0.349	-6.56E-05
	min	0.951	0	mz	0.951	0	mz	0.928	0	mz	0.951	0	mz	0.439	0
	max	2.093	0.0774	min	1.421	-0.00468	max	1.371	0.006298	min	1.421	-0.0632	max	1.06	0.00611
	min	3.549	0	mz	1.766	0	mz	1.693	0	mz	1.766	0	mz	1.318	0
	max	6.537	0.2031	max	2.78	0.03177	min	2.605	-0.0416	max	2.78	0.4289	min	2.12	-0.06829
				mz	3.549	0	mz	3.268	0	mz	3.549	0	mz	2.561	0
				min	4.713	-0.06235	max	4.292	0.0901	min	4.713	-0.8417	max	3.739	0.483
				mz	5.734	0	mz	5.137	0	mz	5.734	0	mz	4.5	0
				max	8.433	0.22358	min	7.112	-0.3219	max	8.433	3.0183	min	6.237	-2.081
							mz	9.425	0				mz	7.682	0
						max	11.617	0.1697				max	10.494	4.508	
2p	max	2	0.3907	min	0.775	-0.0036	max	0.738	0.0049	min	0.775	-0.018	max	0.5222	3.922E-04
				mz	1	0	mz	0.944	0	mz	1	0	mz	0.634	0
				max	3.225	0.3272	min	2.628	-0.3779	max	3.225	1.636	min	1.87	-0.166
							mz	4.027	0				mz	2.366	0
						max	5.419	0.2253				max	4.608	2.262	
3p	max	1.5	0.0802	min	0.6888	-0.00033	max	0.6753	0.000464	min	0.6888	-0.0042	max	0.4746	3.604E-05
	min	3	0	mz	0.879	0	mz	0.8588	0	mz	0.879	0	mz	0.5729	0
	max	6	0.2036	max	2.231	0.0235	min	2.101	-0.0308	max	2.231	0.2942	min	1.56	-0.01474
				mz	3	0	mz	2.778	0	mz	3	0	mz	1.902	0
				min	4.158	-0.0493	max	3.797	0.0688	min	4.158	-0.6167	max	3.218	0.269
				mz	5.121	0	mz	4.599	0	mz	5.121	0	mz	3.927	0
				max	7.922	0.2174	min	6.653	-0.2995	max	7.922	2.717	min	5.723	-1.533
							mz	8.968	0				mz	7.098	0
						max	11.183	0.1631				max	10.024	4.031	
3d	max	4.5	0.2142	min	2.379	-0.00742	max	2.223	0.00247	min	2.379	-0.078	max	1.739	0.004464
				mz	3	0	mz	2.772	0	mz	3	0	mz	2.073	0
				max	6.621	0.19557	min	5.489	-0.05936	max	6.621	2.053	min	4.361	-0.4193
							mz	7.836	0				mz	5.427	0
						max	10.148	0.03622				max	8.9	2.886	

Table S3

Characteristic points for the nuclear charge $Z=3$; max – maximum, min – minimum, mz – zero point
Distance r in a.u.

Z=3	Type	r	$\rho(r)$	Type	r	$f(r)$	Type	r	$df(r)/dN$	Type	r	$s(r)$	Type	r	$ds(r)/dN$
1s	max	0.333	1.624	max	0.667	1.1722	min	0.527	-0.7198	max	0.667	0.7815	min	0.258	-0.0119
							mz	0.93	0				mz	0.333	0
							max	1.333	0.4001				max	1.075	1.0905
2s	max	0.255	0.1558	max	0.453	0.0232	min	0.434	-0.0315	max	0.453	0.062	min	0.2371	-3.424E-04
	min	0.667	0	mz	0.667	0	mz	0.631	0	mz	0.667	0	mz	0.2991	0
	max	1.745	0.5729	min	1.045	-0.0645	max	0.966	0.0855	min	1.045	-0.172	max	0.754	0.034
				mz	1.333	0	mz	1.214	0	mz	1.333	0	mz	0.951	0
				max	2.502	0.5264	min	2.069	-0.6419	max	2.502	1.404	min	1.639	-0.404
							mz	2.995	0				mz	2.083	0
						max	3.896	0.3522				max	3.37	1.925	
3s	max	0.247	0.0445	max	0.435	0.00286	min	0.427	-0.00393	max	0.435	0.0172	min	0.233	-4.38E-05
	min	0.634	0	mz	0.634	0	mz	0.619	0	mz	0.634	0	mz	0.293	0
	max	1.395	0.116	min	0.948	-0.00703	max	0.914	0.009447	min	0.948	-0.0422	max	0.707	0.00407
	min	2.366	0	mz	1.177	0	mz	1.129	0	mz	1.177	0	mz	0.879	0
	max	4.358	0.3046	max	1.853	0.04765	min	1.736	-0.0624	max	1.853	0.2859	min	1.413	-0.04553
				mz	2.366	0	mz	2.179	0	mz	2.366	0	mz	1.707	0
				min	3.142	-0.09353	max	2.861	0.1352	min	3.142	-0.5612	max	2.493	0.322
				mz	3.823	0	mz	3.425	0	mz	3.823	0	mz	3	0
				max	5.622	0.3354	min	4.741	-0.4829	max	5.622	2.0122	min	4.158	-1.387
							mz	6.284	0				mz	5.121	0
						max	7.745	0.2545				max	6.996	3.005	
2p	max	1.333	0.5861	min	0.517	-0.0053	max	0.492	0.0074	min	0.517	-0.0119	max	0.3481	2.614E-04
				mz	0.667	0	mz	0.63	0	mz	0.667	0	mz	0.4226	0
				max	2.15	0.4907	min	1.752	-0.5669	max	2.15	1.0905	min	1.247	-0.111
							mz	2.685	0				mz	1.577	0
						max	3.613	0.3379				max	3.072	1.508	
3p	max	1	0.1203	min	0.4592	-0.0005	max	0.4502	0.000697	min	0.4592	-0.00278	max	0.3164	2.403E-05
	min	2	0	mz	0.586	0	mz	0.5725	0	mz	0.586	0	mz	0.382	0
	max	4	0.3053	max	1.488	0.0353	min	1.401	-0.0462	max	1.488	0.1962	min	1.04	-0.00982
				mz	2	0	mz	1.852	0	mz	2	0	mz	1.268	0
				min	2.772	-0.074	max	2.531	0.1032	min	2.772	-0.4111	max	2.146	0.18
				mz	3.414	0	mz	3.066	0	mz	3.414	0	mz	2.618	0
				max	5.281	0.3261	min	4.436	-0.4492	max	5.281	1.8117	min	3.816	-1.022
							mz	5.979	0				mz	4.732	0
							max	7.456	0.2447				max	6.683	2.687
3d	max	3	0.3212	min	1.586	-0.01113	max	1.482	0.00371	min	1.586	-0.0519	max	1.159	0.002976
				mz	2	0	mz	1.848	0	mz	2	0	mz	1.382	0
				max	4.414	0.29335	min	3.66	-0.08904	max	4.414	1.369	min	2.907	-0.2795
							mz	5.224	0				mz	3.618	0
						max	6.765	0.05433				max	5.933	1.924	